

6-Mercaptopurine
50-44-2 | DTXSID0020810

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.70e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.53e-01

Confidence level: 4.86e-01

Nearest Neighbors from the Training Set

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